Corrected Draft 8 September 2006

The on-shell self-energy of the uniform electron gas in its weak-correlation limit

P. Ziesche

Max-Planck-Institut für Physik komplexer Systeme
Nöthnitzer Str. 38, D-01187 Dresden, Germany

PACS 71.10.Ca, 05.30.Fk

The ring-diagram partial summation (or RPA) for the ground-state energy of the uniform electron gas (with the density parameter r_s) in its weak-correlation limit $r_s \to 0$ is revisited. It is studied, which treatment of the self-energy $\Sigma(k,\omega)$ is in agreement with the Hugenholtz-van Hove (Luttinger-Ward) theorem $\mu - \mu_0 = \Sigma(k_{\rm F},\mu)$ and which is not. The correlation part of the lhs has the RPA asymptotics $a \ln r_s + a' + O(r_s)$ [in atomic units]. The use of renormalized RPA diagrams for the rhs yields the similar expression $a \ln r_s + a'' + O(r_s)$ with the sum rule $a' = a''$ resulting from three sum rules for the components of a' and a''. This includes in the second order of exchange the sum rule $\mu_{2\rm x} = \Sigma_{2\rm x}$ [P. Ziesche, Ann. Phys. (Leipzig), 2006].

I. INTRODUCTION

Although not present in the Periodic Table the uniform or homogeneous electron gas (HEG) is still an important model system for electronic structure theory, cf. e.g. [1]. In its spin-unpolarized version, the HEG ground state is characterized by only one parameter r_s, such that a sphere with the radius r_s contains *on average* one electron [2]. It determines the Fermi wave number as $k_\mathrm{F} = 1/(\alpha r_s)$ in a.u. with $\alpha = [4/(9\pi)]^{1/3} \approx 0.521062$ and it measures simultaneously both the interaction strength and the density such that high density corresponds to weak interaction and hence weak correlation [3]. For recent papers on this limit cf. [4, 5, 6, 7]. Usually the total ground-state energy per particle is written as (here and in the following are wave numbers measured in units of k_F and energies in k_F^2)

$$e = e_0 + e_\mathrm{x} + e_\mathrm{c}, \quad e_0 = \frac{3}{5}\cdot\frac{1}{2}, \quad e_\mathrm{x} = -\frac{3}{4}\cdot\frac{\alpha r_s}{\pi}, \quad e_\mathrm{c} = (\alpha r_s)^2[a \ln r_s + b + b_{2\mathrm{x}} + O(r_s)], \tag{1.1}$$

where e_0 is the energy of the ideal Fermi gas, e_x is the exchange energy in lowest (1st) order, and e_c is referred to as correlation energy given here in its weak-correlation limit with $a = (1 - \ln 2)/\pi^2 \approx 0.031091$ after Macke [9] and $b \approx -0.0711$ after Gell-Mann and Brueckner [10]. e_c contains also the 2nd-order of exchange with $b_{2\mathrm{x}} \approx +0.02418$ after Onsager, Mittag, and Stephen [11]. Notice that $\tilde{e} = k_\mathrm{F}^2 e = e/(\alpha r_s)^2$ gives the energy in a.u., e.g. the energy in zeroth order and the lowest-order exchange energy are $\tilde{e}_0 = 3/(10\ \alpha^2 r_s^2)$ and $\tilde{e}_\mathrm{x} = -3/(4\pi\alpha r_s)$, respectively.

Revisiting how Macke [9], Gell-Mann/Brueckner [10], and Onsager/Mittag/Stephen [11, 12] derived e_c in its weak-correlation limit, it is shown here, that and how an analogous procedure - also called RPA (= random phase approximation) - applies to the self-energy $\Sigma(k,\omega)$. This latter quantity determines (i) the one-body Green's function $G(k,\omega)$, from which follow the quasi-particle dispersion and damping and the momentum distribution $n(k)$ [13]. It furthermore appears (ii) in the Galitskii-Migdal formula for the potential energy [14] (C_+ means the closing of the contour in the upper complex ω-plane),

$$v = \frac{1}{2}\int d(k^3) \int_{C_+} \frac{d\omega}{2\pi \mathrm{i}}\, \mathrm{e}^{\mathrm{i}\omega\delta} G(k,\omega)\Sigma(k,\omega)\ , \quad \delta \underset{\rightarrow}{>} 0\ , \tag{1.2}$$

which is related to the total energy e through the virial theorem [15]

$$v = r_s \frac{d}{dr_s} e\ . \tag{1.3}$$

(iii) Besides, $\Sigma(k,\omega)$ appears in the Luttinger theorem Im $\Sigma(1,\mu) = 0$ [16], in the Hugenholtz-van Hove theorem $\mu - \mu_0 = \Sigma(1,\mu)$ [17], and in the Luttinger-Ward formula for the quasi-particle weight $z_{\rm F}$ [18]:

$$z_{\rm F} = \frac{1}{1-\Sigma'} \ , \quad \Sigma' = \text{Re}\ \frac{\partial\Sigma(1,\omega)}{\partial\omega}\bigg|_{\omega=\mu} \ . \tag{1.4}$$

So $\Sigma(1,\omega)$ is related to the chemical potential μ, which can be calculated from e according to the Seitz theorem [19]

$$\mu = \left(\frac{5}{3} - \frac{1}{3} r_s \frac{d}{dr_s}\right) \ e \ , \tag{1.5}$$

supposed e is known as a function of r_s. Thus from Eq. (1.1) it follows for μ:

$$\mu_0 = \frac{1}{2}, \quad \mu_{\rm x} = -\frac{\alpha r_s}{\pi}, \quad \mu_{\rm c} = (\alpha r_s)^2 \left[a \ln r_s + \left(-\frac{1}{3}a + b + b_{2\rm x}\right) + O(r_s)\right] \ . \tag{1.6}$$

Similarly as in Eqs. (1.1) and (1.6) it is

$$\Sigma(k,\omega) = \Sigma_{\rm x}(k) + \Sigma_{\rm c}(k,\omega), \quad \Sigma_{\rm x}(k) = -\left(1 + \frac{1-k^2}{2k} \ln \left|\frac{k+1}{k-1}\right|\right) \frac{\alpha r_s}{\pi} \ . \tag{1.7}$$

Notice that $\Sigma(k,\omega)$ in lowest order (of exchange) does not depend on ω. In particular, it is $\Sigma_{\rm x}(1) = -\alpha r_s/\pi$, thus $\mu_{\rm x} = \Sigma_{\rm x}(1)$. Similarly, in 2nd order of exchange the sum rule $\mu_{2\rm x} = \Sigma_{2\rm x}(1, \frac{1}{2})$ holds [20]. With $\Sigma_{2\rm x}(1, \frac{1}{2}) = (\alpha r_s)^2 c_{2\rm x}$ it takes the form $b_{2\rm x} = c_{2\rm x}$. The asymptotic behavior $\Sigma_{\rm c}(1,\mu) = (\alpha r_s)^2 [a \ln r_s + c + c_{2\rm x} + O(r_s)]$ and the sum rule

$$-\frac{1}{3}a + b = c \tag{1.8}$$

are a must as a consequence of the Hugenholtz-van Hove theorem. But the question is: which partial summation of Feynman diagrams has to be used for $\Sigma_{\rm c}$ and what has to be used for μ ? The obvious answer to the first question seems to be $\Sigma_{\rm c} = \Sigma_{\rm r} + \cdots$ (the subscript "r" means "ring diagram"). Symbolically written it is defined as $\Sigma_{\rm r} = G_0 \cdot (v_{\rm r} - v_0)$ in terms of the Feynman-diagram building elements G_0, v_0, and $Q(k,\omega)$ [= polarization propagator in RPA], cf. Eqs. (A.2), (A.4), and Fig. 1. $v_{\rm r}$ is the effectively screened Coulomb repulsion following from $v_{\rm r} = v_0 + v_0 Q v_{\rm r}$, see Fig. 2. The Feynman diagrams of $\Sigma_{\rm r}$ are shown in Fig. 3. To what extent this (naive) ansatz has to be changed in a particular way (to answer also the second question) will be discussed at the end of Sec. III.

Naively one should expect that in the weak-correlation limit the Coulomb repulsion ϵ^2/r [3] can be treated as perturbation. But in the early theory of the HEG, Heisenberg [8] has

shown, that ordinary perturbation theory with $e_\mathrm{c} = e_2 + e_3 + \cdots$ and $e_n \sim (\alpha r_s)^n$ does not apply. Namely, in 2nd order, there is a direct term e_2d and an exchange term e_2x, so that $e_2 = e_\mathrm{2d} + e_\mathrm{2x}$. Whereas $e_\mathrm{2x}/(\alpha r_s)^2$, cf. Fig. 4, is a pure finite number b_2x (not depending on r_s), the direct term e_2d logarithmically diverges along the Fermi surface (i.e. for vanishing transition momenta q): $e_\mathrm{2d} \to \ln q$ for $q \to 0$. This failure of perturbation theory has been repaired by Macke [9] with an appropriate partial summation of higher-order terms $e_\mathrm{3r}, e_\mathrm{4r}, \cdots$ (the subscript "r" means "ring diagram") up to infinite order. This procedure replaces the logarithmic divergence for $q \to 0$ by another logarithmic divergence, namely for $r_s \to 0$, cf. Eq. (1.1). This simultaneously "explains", why perturbation theory fails. The coefficient a, first found by Macke [9], has been confirmed later by Gell-Mann and Brueckner [10], who in addition to the logarithmic term numerically calculated two contributions to the next term b, namely b_r and b_2d. More precisely, instead of $e_\mathrm{r} = e_\mathrm{2d} + e_\mathrm{3r} + \cdots$ (notice that $e_\mathrm{2r} = e_\mathrm{2d}$) they calculated a more easily doable approximation $e_\mathrm{r}^0 = e_\mathrm{2d}^0 + e_\mathrm{3r}^0 + \cdots$ (which is sufficient in the weak-correlation limit) with the result $e_\mathrm{r}^0 = (\alpha r_s)^2[a \ln r_s + b_\mathrm{r} + O(r_s)]$, so that $e_\mathrm{r} = e_\mathrm{r}^0 + \Delta e_\mathrm{2d} + O(r_s^3)$ with $\Delta e_\mathrm{2d} = e_\mathrm{2d} - e_\mathrm{2d}^0 = (\alpha r_s)^2 b_\mathrm{2d} + O(r_s^3)$. In summary,

$$
\begin{aligned}
e_\mathrm{c} &= e_\mathrm{r} + e_\mathrm{2x} + O(r_s^3) \\
&= (e_\mathrm{2d} + e_\mathrm{3r} + \cdots) + e_\mathrm{2x} + O(r_s^3) \\
&= (e_\mathrm{2d}^0 + e_\mathrm{3r}^0 + \cdots) + (e_\mathrm{2d} - e_\mathrm{2d}^0) + e_\mathrm{2x} + O(r_s^3) \\
&= e_\mathrm{r}^0 + \Delta e_\mathrm{2d} + e_\mathrm{2x} + O(r_s^3) \\
&= (\alpha r_s)^2\{[a \ln r_s + b_\mathrm{r} + O(r_s)] + b_\mathrm{2d} + b_\mathrm{2x} + O(r_s)\}\ . \qquad (1.9)
\end{aligned}
$$

The result is Eq. (1.1) with $b = b_\mathrm{r} + b_\mathrm{2d}$. This procedure is revisited in Sec. 2 and then in Sec. 3 applied *mutatis mutandis* to the on-the-chemical-potential-shell self-energy $\Sigma(1,\mu)$, the rhs of the Hugenholtz-van Hove theorem. This is a contribution to the mathematics of the weakly-correlated (high-density) HEG). It concerns the HEG self-energy in RPA, extending and completing the paper [6].

II. THE TOTAL ENERGY

The Heisenberg-Macke story starts with the 2nd-order perturbation theory, $e_2 = e_{2\mathrm{d}} + e_{2\mathrm{x}}$. Its components are the direct (d) term $e_{2\mathrm{d}}$ (with $q_0 \underset{\to}{>} 0$) and the exchange (x) term $e_{2\mathrm{x}}$:

$$e_{2\mathrm{d}} = -(\alpha r_s)^2 \frac{2\cdot 3}{(2\pi)^5} \int\limits_{q>q_0} \frac{d^3q\ d^3k_1\ d^3k_2}{q^4}\ \frac{P}{\boldsymbol{q}\cdot(\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{q})}\ ,\ k_{1,2}<1,\ |\boldsymbol{k}_{1,2}+\boldsymbol{q}|>1\ , \quad (2.1)$$

$$e_{2\mathrm{x}} = +(\alpha r_s)^2 \frac{3}{(2\pi)^5} \int \frac{d^3q\ d^3k_1\ d^3k_2}{q^2\ (\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{q})^2}\ \frac{P}{\boldsymbol{q}\cdot(\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{q})}\ ,\ k_{1,2}<1,\ |\boldsymbol{k}_{1,2}+\boldsymbol{q}|>1\ . \quad (2.2)$$

P means the Cauchy principle value. (Notice the prefactor $-1/2$ and the replacement $q^4 \to q^2(\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{q})^2$, when going from $e_{2\mathrm{d}}$ to $e_{2\mathrm{x}}$, and note that the 2nd-order vacuum diagram of Fig. 5 does not contribute.) As already mentioned, the integral (2.2) has been ingeniously calculated by Onsager et al. [11] with the result $e_{2\mathrm{x}} = (\alpha r_s)^2\ b_{2\mathrm{x}}$, $b_{2\mathrm{x}} = \frac{1}{6}\ln 2 - \frac{3}{4}\frac{\zeta(3)}{\pi^2} \approx +0.0242$. Unlike $e_{2\mathrm{x}}$, the direct term $e_{2\mathrm{d}}$ logarithmically diverges for $q_0 \to 0$, i.e. along the Fermi surface. This is seen from

$$e_{2\mathrm{d}} = -(\alpha r_s)^2 \frac{2\cdot 3}{(2\pi)^5} \int\limits_{q>q_0} \frac{d^3q}{q^4} I(q)\ , \quad (2.3)$$

where the Pauli principle makes the function

$$I(q) = \int \frac{d^3k_1\ d^3k_2\ P}{\boldsymbol{q}\cdot(\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{q})}, \quad k_{1,2}<1, \quad |\boldsymbol{k}_{1,2}+\boldsymbol{q}|>1 \quad (2.4)$$

to linearly behave as $I(q\to 0) = \dfrac{8\pi^4}{3} a\ q + O(q^3)$, see App. C, Eq. (C.2). Thus $e_{2\mathrm{d}} = (\alpha r_s)^2[a \ln q_0^2 + \cdots]$, what agrees with (1.1) for $q_0^2 \sim r_s$. The ring-diagram (or RPA) partial summation of Macke [9] and Gell-Mann/Brueckner [10] replaces the artificial (by hand) cut-off q_0 by a natural cut-off $q_c \sim \sqrt{r_s}$. This is made replacing the divergent direct term $e_{2\mathrm{d}}$ by the non-divergent ring-diagram sum

$$e_\mathrm{r} = -\frac{3}{16\pi} \int d^3q \int \frac{d\eta}{2\pi\mathrm{i}} \sum_{n=2}^{\infty} \frac{(-1)^n}{n} \left[\left(\frac{q_c}{q}\right)^2 Q(q,\eta)\right]^n, \quad q_c = \sqrt{\frac{4\alpha r_s}{\pi}}\ . \quad (2.5)$$

For $Q(q,\eta)$, the polarization function in lowest order, is given in Eq. (A.4). With $\eta = \mathrm{i}qu$ the contour integration along the real axis is turned to the imaginary axis:

$$e_\mathrm{r} = \frac{3}{8\pi} \int du \int\limits_0^\infty d(q^2) \left[q^2 \ln\left(1+\frac{q_c^2}{q^2}\right) R(q,u) - q_c^2 R(q,u)\right]\ . \quad (2.6)$$

This has the advantage, that $R(q,u) = Q(q, iqu)$ is a real function, being symmetric in u, cf. Eq. (A.2). Let us control Eq. (2.6): The small-r_s expansion of the u-integrand starts with $(-1/2)(q_c/q)^4 R^2(q,u)$, which just reproduces the 2nd-order direct term $e_{2\mathrm{d}}$ with the help of the integral identity (C.7). For $r_s \to 0$, a direct numerical investigation of Eq. (2.6) yields $e_\mathrm{r} \to (\alpha r_s)^2(0.031091 \ln r_s - 0.0711 + \cdots)$. This result is analytically rederived in the following.

Namely, in the weak-correlation limit $r_s \to 0$ one can approximate $R(q,u) \approx \Theta(q_1 - q)R_0(u) + \cdots$ with $R_0(u) = 1 - u \arctan 1/u$, so that $e_\mathrm{r} = e_\mathrm{r}^0 + O(r_s^3)$, where e_r^0 contains only the q-independent $R_0(u)$ and its q-integration is restricted to $0 \le q \le q_1$:

$$\begin{aligned} e_\mathrm{r}^0 &= \frac{3}{8\pi}\int_0^\infty du \int_0^{q_1} dq^2 \left[q^2 \ln[q^2 + q_c^2 R_0(u)] - q^2 \ln q^2 - q_c^2 R_0(u)\right] \\ &= \frac{3}{8\pi}\int_0^\infty du\, \frac{1}{2} q_c^4 R_0^2(u) \left[\ln\left(\frac{q_c^2}{q_1^2} R_0(u)\right) - \frac{1}{2}\right] + O(r_s^3). \end{aligned} \tag{2.7}$$

(For a discussion of the divergent/convergent behavior of the q-series cf. [10], text after their Eq. (23).) With $q_c^2 = 4\alpha r_s/\pi$ it is

$$e_\mathrm{r}^0 = (\alpha r_s)^2 \frac{3}{\pi^3}\int_0^\infty du\, R_0^2(u) \left[\ln r_s + \ln\frac{4\alpha}{\pi} - \frac{1}{2} + \ln R_0(u) - 2\ln q_1\right] + O(r_s^3). \tag{2.8}$$

So it results $e_\mathrm{r}^0 = (\alpha r_s)^2[a \ln r_s + b_\mathrm{r} - 2a \ln q_1 + O(r_s^3)]$ with

$$\begin{aligned} \frac{3}{\pi^3}\int_0^\infty du\, R_0^2(u) &= a \approx 0.031091\ , \\ b_\mathrm{r} = a\left(\ln\frac{4\alpha}{\pi} - \frac{1}{2}\right) + \frac{3}{\pi^3}\int_0^\infty du\, R_0^2(u) \ln R_0(u) &\approx -0.045423\ . \end{aligned} \tag{2.9}$$

For the integrals cf. Eq. (B.3).

As it has been explained before and in Eq. (1.9), the difference between the correct 2nd-order term of Eq. (2.3) and the first term in the expansion of e_r^0, namely

$$e_{2\mathrm{d}}^0 = -(\alpha r_s)^2\ \frac{2\cdot 3}{\pi^3}\int_{q_0}^{q_1}\frac{dq}{q}\int_0^\infty du\, R_0^2(u) + O(r_s^3) = -(\alpha r_s)^2\ 2a \int_{q_0}^{q_1}\frac{dq}{q} + O(r_s^3)\ , \tag{2.10}$$

gives

$$\Delta e_{2\mathrm{d}} = e_{2\mathrm{d}} - e_{2\mathrm{d}}^0\ =\ -(\alpha r_s)^2\ \frac{2\cdot 3}{\pi^3}\left[\int_{q_0}^{\infty}\frac{dq}{q}\frac{I(q)}{8\pi q} - \left(\int_{q_0}^{1} + \int_1^{q_1}\right)\frac{dq}{q}\frac{\pi^3}{3}a\right] + O(r_s^3) \tag{2.11}$$

$$= (\alpha r_s)^2 \left\{ -\frac{3}{4\pi^4} \left[\int\limits_{q_0}^{1} \frac{dq}{q} \left[\frac{I(q)}{q} - \frac{8\pi^4}{3} a \right] + \int\limits_{1}^{\infty} \frac{dq}{q} \frac{I(q)}{q} \right] + 2a \int\limits_{1}^{q_1} \frac{dq}{q} \right\} + O(r_s^3) \ .$$

$\Delta e_{\rm 2d} = (\alpha r_s)^2[b_{\rm 2d} + 2a \ln q_1 + O(r_s)]$ shows, that the sum $e_{\rm r}^0 + \Delta e_{\rm 2d}$ does not depend on q_1 for $r_s \to 0$. Besides, the first term of $b_{\rm 2d}$ is no longer divergent with $q_0 \to 0$, therefore it can be set $q_0 = 0$:

$$\begin{aligned} b_{\rm 2d} &= -\frac{3}{4\pi^4} \int\limits_{0}^{1} \frac{dq}{q} \left[\frac{I(q)}{q} - \frac{8\pi^4}{3} a \ \Theta(1-q) \right] \\ &= \frac{1}{4} + \frac{1}{\pi^2} \left[-\frac{11}{6} - \frac{8}{3} \ln 2 + 2(\ln 2)^2 \right] \approx -0.025677 \ . \end{aligned} \tag{2.12}$$

Together it is $b = b_{\rm r} + b_{\rm 2d} \approx -0.0711$, what agrees with the above mentioned numerical evaluation of Eq. (2.6).

III. THE SELF-ENERGY

Here - after the training of Sec. II - , it is aimed to calculate $\Sigma_{\rm c}(1, \mu)$ in the weak-correlation limit, where there is a scheme for $\Sigma_{\rm c}(1, \mu)$ analog to Eq. (1.9) for $e_{\rm c}$ with one difference. Namely, whereas the chemical-potential shift μ results from vacuum diagrams, the self-energy $\Sigma(k, \omega)$ results from non-vacuum diagrams, which are functions of k and ω, see the discussion at the end of this Section.

In analogy to Eqs. (2.1) and (2.2), the self-energy in 2nd order is $\Sigma_2(k, \omega) = \Sigma_{\rm 2d}(k, \omega) + \Sigma_{\rm 2x}(k, \omega)$, the 2nd-order self-energy diagram of Fig. 5 vanishes. From (A.6) it follows for the direct term

$$\begin{aligned} \Sigma_{\rm 2d}(1, \omega) = \frac{(\alpha r_s)^2}{2\pi^4} \int\limits_{q>q_0} \frac{d^3q d^3k_2}{q^4} & \left[\frac{\Theta(|\boldsymbol{e}_1 + \boldsymbol{q}| - 1)}{\omega - \frac{1}{2} - \boldsymbol{q} \cdot (\boldsymbol{e}_1 + \boldsymbol{k}_2 + \boldsymbol{q}) + {\rm i}\delta} \right. \\ & \left. + \frac{\Theta(1 - |\boldsymbol{e}_1 + \boldsymbol{q}|)}{\omega - \frac{1}{2} - \boldsymbol{q} \cdot (\boldsymbol{e}_1 - \boldsymbol{k}_2) - {\rm i}\delta} \right] \Theta(1 - k_2) \Theta(|\boldsymbol{k}_2 + \boldsymbol{q}| - 1). \end{aligned} \tag{3.1}$$

For the corresponding exchange term $\Sigma_{\rm 2x}(1, \omega)$ cf. Fig. 4 and ref. [20], where it has been shown that $\Sigma_{\rm 2x} = {\rm Re}\ \Sigma_{\rm 2x}(1, \frac{1}{2}) = (\alpha r_s)^2 c_{\rm 2x}$ with the sum rule $c_{\rm 2x} = b_{\rm 2x} \approx +0.0242$. On the other hand, the direct term $\Sigma_{\rm 2d}$ diverges logarithmically for $q_0 \to 0$. This is seen from

$$\Sigma_{\rm 2d} = {\rm Re}\ \Sigma_{\rm 2d} \left(1, \frac{1}{2}\right) = -\frac{(\alpha r_s)^2}{2\pi^4} \int\limits_{q>q_0} \frac{d^3q}{q^4} J(q) \ , \tag{3.2}$$

where the Pauli principle makes the function

$$J(q)=\int\frac{d^2e_1}{4\pi}d^3k_2\left[\frac{\Theta(|\boldsymbol{e}_1+\boldsymbol{q}|-1)P}{\boldsymbol{q}\cdot(\boldsymbol{e}_1+\boldsymbol{k}_2+\boldsymbol{q})}+\frac{\Theta(1-|\boldsymbol{e}_1+\boldsymbol{q}|)P}{\boldsymbol{q}\cdot(\boldsymbol{e}_1-\boldsymbol{k}_2)}\right]\Theta(1-k_2)\Theta(|\boldsymbol{k}_2+\boldsymbol{q}|-1)\ ,\tag{3.3}$$

to linearly behave as $J(q\to 0)=\pi^3 a\ q+O(q^3)$, see App. D, Eq. (D.2). Thus $\Sigma_{\rm 2d}=(\alpha r_s)^2(a\ln q_0^2+\cdots)$, what is for $q_0^2\sim r_s$ in full agreement with the Hugenholtz-van Hove theorem (1.4) and the perturbation expansion of μ, which - because of (1.5) - gives $\mu_{\rm 2d}=e_{\rm 2d}=(\alpha r_s)^2(a\ln r_s+\cdots)$. In the ring-diagram partial summation the divergent direct term $\Sigma_{\rm 2d}(k,\omega)$ is replaced by the non-divergent sum (its Feynman diagrams are shown in Fig. 3)

$$\begin{aligned}\Sigma_{\rm r}(k,\omega)\ &=\ (\alpha r_s)^2\ \frac{2}{\pi^3}\int\frac{d^3q}{q^2}\int\frac{d\eta}{2\pi\mathrm{i}}\ \frac{Q(q,\eta)}{q^2+q_c^2Q(q,\eta)}\ \times\\ &\times\ \left[\frac{\Theta(|\boldsymbol{k}+\boldsymbol{q}|-1)}{\omega+\eta-\frac{1}{2}k^2-\boldsymbol{q}\cdot(\boldsymbol{k}+\frac{1}{2}\boldsymbol{q})+\mathrm{i}\delta}+\frac{\Theta(1-|\boldsymbol{k}+\boldsymbol{q}|)}{\omega+\eta-\frac{1}{2}k^2-\boldsymbol{q}\cdot(\boldsymbol{k}+\frac{1}{2}\boldsymbol{q})-\mathrm{i}\delta}\right].\end{aligned}\tag{3.4}$$

Next, this expression is carefully controlled:
(i) If the term $q_c^2Q(q,\eta)$, which describes the RPA screening of the bare Coulomb interaction $1/q^2$, is deleted, then $\Sigma_{\rm r}(k,\omega)$ changes to $\Sigma_{\rm 2d}(k,\omega)$, as it is seen from Eq. (A.5).
(ii) Use of Eq. (3.4) in the Galitskii-Migdal formula (1.2) yields the ring-diagram summation for the potential energy, $v_{\rm r}$, which follows from $e_{\rm r}$ through the virial theorem (1.3).
(iii) The expression (3.4) allows to calculate the derivative $\Sigma'_{\rm r}(k,\omega)=\partial\Sigma_{\rm r}(k,\omega)/\partial\omega$. From $\Sigma'_{\rm r}=\mathrm{Re}\ \Sigma'_{\rm r}(1,\frac{1}{2})$ one obtains $z_{\rm F}$ in RPA by means of the Luttinger-Ward formula (1.4) as $z_{\rm F}=1+\Sigma'_{\rm r}+\cdots$ with

$$\Sigma'_{\rm r}=\frac{\alpha r_s}{\pi^2}\int\limits_0^\infty du\ \frac{R'_0(u)}{R_0(u)}\arctan\frac{1}{u}+\cdots=-0.177038\ r_s+\cdots\ .\tag{3.5}$$

This is just the well-known RPA result for $z_{\rm F}$ [24]. For the integral see Eq. (B.4).

After this controlling and training, $\Sigma_{\rm r}=\mathrm{Re}\ \Sigma_{\rm r}(1,\frac{1}{2})$ is derived from Eq. (3.4) in a similar way as $e_{\rm r}$ in Eqs. (2.7) - (2.12). The next steps again are substitution $\eta=\mathrm{i}qu$ and contour deformation from the real to the imaginary axis with $x=\boldsymbol{e}\cdot\boldsymbol{e}_q$ and $|\boldsymbol{e}+\boldsymbol{q}|\gtrless 1\pm\delta$:

$$\begin{aligned}\Sigma_{\rm r}\ &=\ -\frac{(\alpha r_s)^2}{\pi^4}\int\frac{d^3q}{q^2}\int du\ \frac{R(q,u)}{q^2+q_c^2R(q,u)}\cdot\frac{1}{(x+\frac{q}{2})-\mathrm{i}u}\\ &=\ -\frac{(\alpha r_s)^2}{\pi^4}\int\limits_0^\infty du\ \int\frac{d^3q}{q^2}\ \frac{R(q,u)}{q^2+q_c^2R(q,u)}\cdot\frac{2(x+\frac{q}{2})}{(x+\frac{q}{2})^2+u^2}\ .\end{aligned}\tag{3.6}$$

In the last step the u- and $\boldsymbol{q}$-integrations are exchanged and it is used that $R(q,u)$ is even in u, cf. Eq. (B.1); so the imaginary part again vanishes. Next the $\boldsymbol{q}$-integration is specified as

$$\begin{aligned}\Sigma_{\mathrm{r}} &= -\frac{(\alpha r_s)^2}{\pi^4}\int_0^\infty du \int \frac{d^3q}{q^2}\,\frac{R(q,u)}{q^2+q_c^2R(q,u)}\cdot\int_{-1}^{+1}\frac{dx}{2}\,\frac{2(x+\frac{q}{2})}{(x+\frac{q}{2})^2+u^2}\\ &= -(\alpha r_s)^2\frac{2}{\pi^3}\int_0^\infty du\int_0^\infty dq\,\frac{R(q,u)}{q^2+q_c^2R(q,u)}\cdot\ln\frac{(\frac{q}{2}+1)^2+u^2}{(\frac{q}{2}-1)^2+u^2}\ .\end{aligned}\qquad(3.7)$$

Let us control Eq. (3.7): The small-r_s expansion of the u-integrand starts with $R(q,u)/q^2$, which just reproduces the 2nd-order direct term (3.3) with the help of the integral identity (D.7). In the limit $r_s\to 0$, Eq. (3.7) numerically gives $\Sigma_{\mathrm{r}}\approx(\alpha r_s)^2(0.031091\ln r_s - 0.081463+\cdots)$. This result is analytically confirmed by the following. The asymptotic behavior for $r_s\to 0$ is determined by the lower integration limit $q\to 0$, therefore $R(q,u)$ and $\ln\cdots$ can be approximated by $R_0(u) = 1-u\arctan 1/u$ and $L_0(u)=2q/(1+u^2)$, respectively:

$$\Sigma_{\mathrm{r}} = -(\alpha r_s)^2\frac{2}{\pi^3}\int_0^\infty du\int_0^\infty d(q^2)\,\frac{[R_0(u)+R_1(u)q^2+\cdots][L_0(u)+L_1(u)q^2+\cdots]}{q^2+q_c^2[R_0(u)+R_1(u)q^2+\cdots]} = \Sigma_{\mathrm{r}}^0 + O(r_s^3)\ . \qquad(3.8)$$

Finally the q-integration yields

$$\begin{aligned}\Sigma_{\mathrm{r}}^0 &= -(\alpha r_s)^2\frac{2}{\pi^3}\int_0^\infty du\,\frac{R_0(u)}{1+u^2}\int_0^{q_2}\frac{dq^2}{q^2+q_c^2R_0(u)}\\ &= -(\alpha r_s)^2\frac{2}{\pi^3}\int_0^\infty du\,\frac{R_0(u)}{1+u^2}\,\ln[q^2+q_c^2R_0(u)]\Big|_0^{q_2}\\ &= -(\alpha r_s)^2\frac{2}{\pi^3}\int_0^\infty du\,\frac{R_0(u)}{1+u^2}\,[2\ln q_2-\ln q_c^2R_0(u)]\ .\end{aligned}\qquad(3.9)$$

With Eq. (B.3) it turns out $\Sigma_{\mathrm{r}}^0 = (\alpha r_s)^2[a\ln r_s + c_{\mathrm{r}} - 2a\ln q_2 + O(r_s)]$,

$$c_{\mathrm{r}} = a\ln\frac{4\alpha}{\pi}+\frac{2}{\pi^3}\int_0^\infty du\,\frac{R_0(u)\ln R_0(u)}{1+u^2}\approx -0.035059\ . \qquad(3.10)$$

The difference between the exact 2nd-order term of Eq. (3.2) and the first term in the q-expansion of Σ_{r}^0, namely

$$\Sigma_{\mathrm{2d}}^0 = -(\alpha r_s)^2\frac{2}{\pi^3}\int_{q_0}^{q_2}\frac{dq}{q^2}\int_0^\infty du\;R_0(u)\;\frac{2q}{1+u^2} = -(\alpha r_s)^2\frac{2}{\pi^3}\int_{q_0}^{q_2}\frac{dq}{q}\pi(1-\ln 2)\ , \qquad(3.11)$$

yields

$$\begin{aligned}\Delta\Sigma_{2\mathrm{d}} = \Sigma_{2\mathrm{d}} - \Sigma_{2\mathrm{d}}^0 &= -(\alpha r_s)^2 \frac{2}{\pi^3}\left[\int_{q_0}^{\infty} \frac{dq}{q}\frac{J(q)}{q} - \int_{q_0}^{q_2} \frac{dq}{q}\pi(1-\ln 2)\right] \qquad (3.12)\\ &= (\alpha r_s)^2 \left\{-\frac{2}{\pi^3}\left[\int_{q_0}^{1}\frac{dq}{q}\left[\frac{J(q)}{q} - \pi(1-\ln 2)\right] + \int_1^{\infty}\frac{dq}{q}\frac{J(q)}{q}\right] + 2a\int_1^{q_2}\frac{dq}{q}\right\}\ .\end{aligned}$$

$\Delta\Sigma_{2\mathrm{d}} = (\alpha r_s)^2[c_{2\mathrm{d}} + 2a\ln q_2 + \cdots]$ shows, that the sum $\Sigma_{\mathrm{r}}^0 + \Delta\Sigma_{2\mathrm{d}}$ does not depend on q_2 for $r_s \to 0$. Besides the first term of $c_{2\mathrm{d}}$ is no longer divergent with $q_0 \to 0$, therefore it can be set $q_0 = 0$:

$$c_{2\mathrm{d}} = -\frac{2}{\pi^3}\int_0^{\infty}\frac{dq}{q}\left[\frac{J(q)}{q} - \pi(1-\ln 2)\Theta(1-q)\right] \approx -0.046404\ . \qquad (3.13)$$

For the $J(q)$-integral cf. Eq. (D.4). Together it is $c = c_{\mathrm{r}} + c_{2\mathrm{d}} \approx -0.08146$, to be compared with $-\frac{1}{3}a + b = -0.08146$. This is just the expected sum rule (1.8). But the difference $\Sigma_{\mathrm{r}}(1, \frac{1}{2} + \mu_{\mathrm{x}}\cdots) - \Sigma_{\mathrm{r}}(1, \frac{1}{2}) \neq 0$ seems to disturb this sum rule $c = -\frac{1}{3}a + b$. This 'misfit' is removed by an additional partial summation replacing Fig. 3 by Fig. 6, i.e. replacing $\Sigma_{\mathrm{r}} = G_0 \cdot (v_{\mathrm{r}} - v_0)$ by $\Sigma_{\mathrm{r}}^{\mathrm{x}} = G_{\mathrm{x}} \cdot (v_{\mathrm{r}} - v_0)$ with the renormalized one-body Green's function

$$G_{\mathrm{x}}(k,\omega) = \frac{1}{\omega - \frac{1}{2}k^2 - \Sigma_{\mathrm{x}}(k) \pm \mathrm{i}\delta}\ , \qquad (3.14)$$

see Fig. 7. For $k = 1$ it is $G_{\mathrm{x}}(1,\omega) = 1/[\omega - \frac{1}{2} - \mu_{\mathrm{x}} \pm \mathrm{i}\delta]$. Thus $\Sigma_{\mathrm{r}}^{\mathrm{x}}(1, \frac{1}{2} + \mu_{\mathrm{x}} + \cdots) = \Sigma_{\mathrm{r}}(1, \frac{1}{2}) + \cdots$ in the limit $r_s \to 0$. So the conjectured relation (1.8) holds. This can be seen still in another way.

Namely, note the similarities of Eqs. (3.10) and (2.9) as well as Eqs. (3.13) and (2.12). Their differences are

$$c_{\mathrm{r}} - b_{\mathrm{r}} = \frac{1}{3}a \quad \text{and} \quad c_{2\mathrm{d}} - b_{2\mathrm{d}} = -\frac{2}{3}a \qquad (3.15)$$

using the identities (B.5) and (D.8), respectively. Thus, with $b = b_{\mathrm{r}} + b_{2\mathrm{d}}$ and $c = c_{\mathrm{r}} + c_{2\mathrm{d}}$, the sum rule (1.8) is proven once more.

IV. SUMMARY

Summarizing, the Hugenholtz-van Hove theorem $\mu - \mu_0 = \Sigma(1,\mu)$ takes for the HEG ground state in its weak-correlation limit $r_s \to 0$ the asymptotic form

$$-\frac{\alpha r_s}{\pi} + (\alpha r_s)^2[a\ln r_s + \left(-\tfrac{1}{3}a + b_{\mathrm{r}} + b_{2\mathrm{d}}\right) + b_{2\mathrm{x}} + O(r_s)] =$$

$$-\frac{\alpha r_s}{\pi} + (\alpha r_s)^2[a \ln r_s + \quad (c_\mathrm{r} + c_\mathrm{2d}) \quad + c_\mathrm{2x} + O(r_s)] \ . \tag{4.1}$$

So the sum rules [with $a = \frac{1}{\pi^2}(1 - \ln 2)$ and $b_\mathrm{r}, b_\mathrm{2d}, c_\mathrm{r}, c_\mathrm{2d}$ given in Eqs. (2.9), (2.12), (3.10), (3.13)]

$$\frac{1}{3}a + b_\mathrm{r} = c_\mathrm{r}, \quad -\frac{2}{3}a + b_\mathrm{2d} = c_\mathrm{2d}, \quad b_\mathrm{2x} = c_\mathrm{2x} \tag{4.2}$$

hold. The last relation or $\mu_\mathrm{2x} = \Sigma_\mathrm{2x}$ has been shown in [20]. The sum rules (4.2) are relations between the Macke number a, the Gell-Mann/Brueckner numbers b_r, b_2d and the Onsager/Mittag/Stephen number b_2x (which altogether desribe the $r_s \to 0$ asymptotics of the correlation energy e_c) on the one hand and corresponding numbers c_r, c_2d, c_2x of the on-shell self-energy $\Sigma(1, \mu)$ on the other hand. Eqs. (4.1) and (4.2) answer the question which partial summation of Feynman diagrams has to be used in the weak-correlation limit for the self-energy Σ on the rhs of the Hugenholtz-van Hove theorem. They result from the renormalized ring-diagram (or RPA) partial summation (symbolically written as) $\Sigma \approx \Sigma_\mathrm{r}^\mathrm{x} = G_\mathrm{x} \cdot v_\mathrm{r}$ with $v_\mathrm{r} = v_0/(1 - Qv_0)$ and $G_\mathrm{x}(k, \omega) =$ renormalized one-body Green's function and $Q(q, \eta) =$ polarization propagator in RPA, see Eqs. (3.14) and (A.4), respectively, and Figs. 1, 2, 6, 7. (They not result from $\Sigma \approx \Sigma^\mathrm{HF} = G \cdot v_0$, see Fig. 8, as an alternative ansatz with $G(k, \omega) =$ full one-body Green's function of the interacting system [21].) Byproducts are the analytical representation of b_2d, a detailed description of the momentum-transfer or Macke function $I(q)$ for the RPA vacuum diagrams (App. C), the introduction and discussion of an analog function $J(q)$ for the RPA self-energy diagrams (App. D), and the proof of integral identities, which relate $I(q)$ and $J(q)$ to the polarization-propagator function $R(q, u)$, cf. Apps. C and D.

Acknowledgments

The author thanks G. Diener and E. Runge for valuable hints and F. Tasnádi for technical help and acknowledges P. Fulde for supporting this work.

---

[1] M.P. Tosi in: N.H. March (Ed.), *Electron Correlation in the Solid State*, Imperial College Press, 1999, p. 1.

[2] There is a non-vanishing probability of finding 0, 2, 3, ... electrons in such a Wigner sphere. Such particle number fluctuations in fragments have been studied by P. Ziesche, J. Tao, M. Seidl, and J.P. Perdew, Int. J. Quantum Chem. **77**, 819 (2000) with the conclusion 'correlation suppresses fluctuations', cf. also P. Fulde, *Electron Correlations in Molecules and Solids*, 3rd ed., Springer, Berlin, 1995, p.157.

[3] The Coulomb repulsion takes the form $\alpha r_s/r$, if lengths and energies are measured in units of k_F^{-1} and k_F^2, respectively. This shows that r_s is not only a density parameter [2], but also the interaction strength. Its Fourier transform is $4\pi\alpha r_s/q^2$ with q measured in units of k_F.

[4] P. Ziesche, Int J. Quantum Chem. **90**, 342 (2002).

[5] P. Ziesche and J. Cioslowski, Physica A **356**, 598 (2005). Here it is shown, which peculiarities of $n(k)$ and $S(q)$ caused by RPA lead to $e_\mathrm{c} \sim r_s^2 \ln r_s$.

[6] J. Cioslowski and P. Ziesche, submitted.

[7] R.D. Muiño, I. Nagy, and P.M. Echenique, Phys. Rev. B **72**, 075117 (2005).

[8] W. Heisenberg, Z. Naturf. **2a**, 185 (1947).

[9] W. Macke, Z. Naturf. **5a**, 192 (1950).

[10] M. Gell-Mann and K. Brueckner, Phys. Rev. **106**, 364 (1957).

[11] L. Onsager, L. Mittag, and M. J. Stephen, Ann. Physik (Leipzig) **18**, 71 (1966). Here the exchange integral of the 3D electron gas has been evaluated *analytically*. This rather herculean work was generalized and extended to the d-dimensional electron gas by M.L. Glasser [12]

[12] M.L. Glasser, J. Comp. Appl. Math. **10**, 293 (1984).

[13] For a recent parametrization of $n(k, r_s)$ see P. Gori-Giorgi and P. Ziesche, Phys. Rev. B **66**, 235116 (2002). Its intention was to provide an *analytical* expression for $n(k, r_s)$ in the range $r_s = 1, \cdots, 10$. In this range $n(k, r_s)$ is carefully fitted to the well-known kinetic energy $t(r_s)$. But numerical inaccurancies in the fitted expressions (17), (18), (19) made, that $n(k, r_s)$ is for $r_s = 0, \cdots, 1$ not accurate enough fo fully recover the well-known RPA behavior for $r_s \gtrsim 0$.

[14] W.M. Galitskii and A.B. Migdal, Zh. Éksp. Teor. Fiz. **34**, 139 (1958) [Sov. Phys. JETP **7**, 96 (1958)].

[15] N.H. March, Phys. Rev. **110**, 604 (1958).

[16] J.M. Luttinger, Phys. Rev. **121**, 942, 1251 (1961)

[17] N.M. Hugenholtz and L. van Hove, Physica **24**, 363 (1958). Their theorem has been brought into the form $\mu - \mu_0 = \Sigma(1, \mu)$ in ref. [18].

[18] J.M. Luttinger and J.C. Ward, Phys. Rev. **118**, 1417 (1960).

[19] F. Seitz, *Modern Theory of Solids*, McGraw-Hill, New York, 1940, Sec. 76.

[20] P. Ziesche, cond-mat/0605188 and Ann. Phys. (Leipzig), in press.

[21] The renormalized ring-diagram partial summation $\Sigma_{\mathrm{r}}^{\mathrm{x}} = G_{\mathrm{x}} \cdot (r_{\mathrm{r}} - v_0)$ yields the correct $r_s \to 0$ asymptotics up to r_s^2, see Eqs. (4.1) and (4.2). Thus all the other remaining diagrams or summations (e.g. $\Sigma_{\mathrm{c}}^{\mathrm{HF}} = (G - G_0)v_0$ of ref. [22]) can contribute only to higher-order asymptotics.

[22] B. Farid, Phil. Mag.**84**, 109 (2004), Eq. (84).

[23] G.G. Hoffman, Phys.Rev. B**45**, 8730 (1992).

[24] E. Daniel and S.H. Vosko, Phys. Rev. **120**, 2041 (1960); I.O. Kulik, Zh. Éksp. teor. **40**, 1343 (1961) [Sov. Phys. JETP **13**, 946 (1961)].

APPENDIX A: ONE-BODY GREEN'S FUNCTION, PARTICLE-HOLE PROPAGATOR, AND 2ND-ORDER SELF-ENERGY

In the following the identities (with $z = x + \mathrm{i}y$)

$$\int\limits_{C_\pm} \frac{dz}{2\pi\mathrm{i}} \frac{1}{(z - z_1)(z - z_2)} = \begin{cases} 0 & \text{for sign } y_1 = \text{sign } y_2 \\ \dfrac{1}{z_1 - z_2} & \text{for } y_1 > 0 \text{ and } y_2 < 0 \\ \dfrac{1}{z_2 - z_1} & \text{for } y_1 < 0 \text{ and } y_2 > 0 \end{cases} \tag{A.1}$$

for contour integrations in the complex z-plane are used ($z = x + \mathrm{i}y$, $C_\pm$= contour along the real axis, closed above or below with a half circle). The building elements of the Feynman diagrams are

$$G_0(k,\omega) = \frac{\Theta(k-1)}{\omega - \frac{1}{2}k^2 + \mathrm{i}\delta} + \frac{\Theta(1-k)}{\omega - \frac{1}{2}k^2 - \mathrm{i}\delta}\ , \quad \delta \underset{\to}{>} 0 \quad \text{and} \quad v_0(q) = \frac{4\pi\alpha r_s}{q^2}\ . \tag{A.2}$$

From G_0 follows the particle-hole propagator Q in RPA according to

$$Q(q,\eta) = -\int \frac{d^3k}{4\pi} \int \frac{d\omega}{2\pi\mathrm{i}} G_0(k,\omega) G_0(|\boldsymbol{k}+\boldsymbol{q}|, \omega+\eta) \tag{A.3}$$

with the result

$$Q(q,\eta) = \int \frac{d^3k}{4\pi} \left[\frac{1}{\boldsymbol{q}(\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}) - \eta - \mathrm{i}\delta} + \frac{1}{\boldsymbol{q}(\boldsymbol{k}+\frac{1}{2}\boldsymbol{q}) + \eta - \mathrm{i}\delta} \right] \Theta(1-k)\Theta(|\boldsymbol{k}+\boldsymbol{q}|-1). \tag{A.4}$$

(A.2) and (A.4) used in the direct term of the 2nd-order off-shell self-energy

$$\Sigma_{2\mathrm{d}}(k,\omega) = (\alpha r_s)^2\ \frac{2}{\pi^3} \int\limits_{q>q_0} \frac{d^3q}{q^4} \int \frac{d\eta}{2\pi\mathrm{i}}\ Q(q,\eta) G_0(|\boldsymbol{k}+\boldsymbol{q}|,\omega+\eta) \tag{A.5}$$

yields

$$\Sigma_{2\mathrm{d}}(k,\omega) = \frac{(\alpha r_s)^2}{2\pi^4} \int\limits_{q>q_0} \frac{d^3q}{q^4} \int d^3k' \ \left[\frac{\Theta(|\boldsymbol{k}+\boldsymbol{q}|-1)}{\omega - \frac{1}{2}k^2 - \boldsymbol{q}\cdot(\boldsymbol{k}+\boldsymbol{k}'+\boldsymbol{q}) + \mathrm{i}\delta} + \frac{\Theta(1-|\boldsymbol{k}+\boldsymbol{q}|)}{\omega - \frac{1}{2}k^2 - \boldsymbol{q}\cdot(\boldsymbol{k}-\boldsymbol{k}') - \mathrm{i}\delta}\right] \ \Theta(1-k')\Theta(|\boldsymbol{k}'+\boldsymbol{q}|-1). \tag{A.6}$$

This expression used in (1.2) yields $v_{2\mathrm{d}} = 2e_{2\mathrm{d}}$ in agreement with the virial theorem (1.3).

APPENDIX B: THE FUNCTION $R(q,u)$

$Q(q,\eta)$ becomes real for imaginary η:

$$R(q,u) = Q(q,\mathrm{i}qu) = \frac{1}{2}\left[1 + \frac{1+u^2-\frac{q^2}{4}}{2q} \ln \frac{(\frac{q}{2}+1)^2+u^2}{(\frac{q}{2}-1)^2+u^2} - u\left(\arctan\frac{1+\frac{q}{2}}{u} + \arctan\frac{1-\frac{q}{2}}{u}\right)\right]. \tag{B.1}$$

The function $R(q,u)$ has the q-expansion $R(q,u) = R_0(u) + q^2 R_1(u) + \cdots$ with

$$R_0(u) = 1 - u\arctan\frac{1}{u}\ , \quad R_1(u) = -\frac{1}{12(1+u^2)^2}\ , \quad R_2(u) = -\frac{1-5u^2}{240(1+u^2)^4}\ . \tag{B.2}$$

Here is a list of integrals:

$$\begin{aligned} \int\limits_0^\infty du\ R_0^2(u) &= \frac{\pi^3}{3}a \approx 0.321336, & \int\limits_0^\infty du\ R_0^2(u)\ln R_0(u) &\approx -0.176945, \\ \int\limits_0^\infty du\ \frac{R_0(u)}{1+u^2} &= \frac{\pi^3}{2}a \approx 0.482003, & \int\limits_0^\infty du\ \frac{R_0(u)\ln R_0(u)}{1+u^2} &\approx -0.345751, \end{aligned} \tag{B.3}$$

$$\int\limits_0^\infty du\ \frac{R_0'(u)}{R_0(u)}\arctan\frac{1}{u} \approx -3.353337\ , \quad \int\limits_0^\infty du\ \frac{R_0''(u)}{R_0(u)}\arctan\frac{1}{u} \approx 4.581817\ . \tag{B.4}$$

The last but one integral appears in the weak-correlation limit of the quasi-particle weight z_F [24]. The identity

$$\frac{2}{\pi^3}\int\limits_0^\infty du\ R_0(u)\ln R_0(u)\left[\frac{1}{1+u^2} - \frac{3}{2}R_0(u)\right] = -\frac{1}{6}a \tag{B.5}$$

leads to the sum rule (3.15).

APPENDIX C: THE FUNCTION $I(q)$

Using cylindrical coordinates and the centre of the vector $\boldsymbol{q}$ as origin, Macke [9] succeeded to calculate $I(q)$ explicitly as

$$
\begin{aligned}
I(q \le 2) = \pi^2 \Bigg[\left(\frac{29}{15} - \frac{8}{3}\ln 2 \right) q - \frac{q^3}{20} &+ \frac{1}{q}\left(\frac{16}{15} + q - \frac{q^3}{6} + \frac{q^5}{80} \right) \ln\left(1+\frac{q}{2}\right) \\
&+ \frac{1}{q}\left(\frac{16}{15} - q + \frac{q^3}{6} - \frac{q^5}{80} \right) \ln\left(1-\frac{q}{2}\right) \Bigg],
\end{aligned}
$$

$$
\begin{aligned}
I(q \ge 2) = \frac{\pi^2}{30}\Big[4\,(22+q^2) &+ \frac{1}{q}(q+2)^3(4-6q+q^2)\ln\left(1+\frac{2}{q}\right) \\
&+ \frac{1}{q}(q-2)^3(4+6q+q^2)\ln\left(1-\frac{2}{q}\right) \Big] .
\end{aligned} \tag{C.1}
$$

Therefore $I(q)$ is referred to as Macke function, cf. also [23]. (The last two lines of (C.1) correct errors in [4], Eq. (A.1).) $I(q)$ has the properties

$$
\begin{aligned}
I(q \to 0) &= \frac{8\pi^2}{3}(1-\ln 2)\, q - \frac{\pi^2}{6}\, q^3 + \cdots, \quad I(q\to\infty) = \left(\frac{4\pi}{3}\right)^2 \left(\frac{1}{q^2} + \frac{2}{5}\frac{1}{q^4} + \cdots \right), \\
I(2) &= \frac{4\pi^2}{15}(13 - 16\ln 2) \approx 5.02598, \quad I'(2) = -\frac{8\pi^2}{5}(-1+2\ln 2) \approx -6.10012, \\
I''(2^+) &= \frac{8\pi^2}{15}(2+\ln 2) \approx 14.1762, \quad I''(2^-) = -\frac{2\pi^2}{15}(7-4\ln 2) \approx -5.56305.
\end{aligned} \tag{C.2}
$$

$I(q)$ has a maximum of 7.12 at $q = 1.36$. $I(q)$ and $I'(q)$ are continuous at $q = 2$, but $I''(q)$ has there a jump discontinuity of $2\pi^2$. This is because the topology changes from overlapping to non-overlapping Fermi spheres, when passing $q = 2$ from below. Its normalization is

$$
\int_0^\infty dq\; I(q) = \frac{8\pi^2}{45}(-3+\pi^2+6\ln 2) \approx 19.3505. \tag{C.3}
$$

$I(q)$ is shown in Fig. 9. Multiplying the integral

$$
\int_0^\infty \frac{dq}{q^2}\left[I(q) - \frac{8\pi^2}{3}(1-\ln 2)\; q\Theta(1-q) \right] = \frac{\pi^2}{9}\left[22 - 3\pi^2 + 32\ln 2 - 24(\ln 2)^2 \right] \approx 3.334856 \tag{C.4}
$$

with $-3/(4\pi^4)$ yields Eq. (2.12).

The original expression for $I(q)$ arises from the diagram rules for $e_{2\mathrm{d}}$ with Eq. (3.3) as

$$
I(q) = \frac{1}{2}(4\pi)^2 \mathrm{Re} \int \frac{d\eta}{2\pi \mathrm{i}}\; Q^2(q,\eta). \tag{C.5}
$$

One way is to insert (A.4) into (C.5). It results (with $x_i = \boldsymbol{q}\cdot(\boldsymbol{k}_i + \frac{1}{2}\boldsymbol{q}), i = 1,2$)

$$I(q) = \mathrm{Re} \int \frac{d^3k_1 d^3k_2}{x_1 + x_2 - \mathrm{i}\delta} = \int \frac{d^3k_1 d^3k_2\ P}{\boldsymbol{q}\cdot(\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{q})} \tag{C.6}$$

in agreement with Eq. (2.4). Another way is the analytical continuation and the deformation of the integration contour from the real to the imaginary axis with the advantage that $R(q,u) = Q(q,\mathrm{i}qu)$ is a real function. This yields

$$I(q) = 2\cdot 4\pi q \int_0^\infty du\ R^2(q,u) \tag{C.7}$$

as an integral identity.

APPENDIX D: THE FUNCTION $J(q)$

Using again the method of Macke yields

$$\begin{aligned} J(q\le 2) = \frac{\pi}{4}q\Big[\frac{8}{3} - 4\ln 2 \ &+\ \frac{1}{3}\left(2-\frac{q}{2}\right)\left(1+\frac{2}{q}\right)^2 \ln\left(1+\frac{q}{2}\right) \\ &+\ \frac{1}{3}\left(2+\frac{q}{2}\right)\left(1-\frac{2}{q}\right)^2 \ln\left(1-\frac{q}{2}\right)\Big], \\ J(q\ge 2) = \frac{4\pi}{3}q\,[1 \ &+\ \frac{1}{8q}(1-q)(2+q)^2 \ln\left(1+\frac{2}{q}\right) \\ &-\ \frac{1}{8q}(1+q)(2-q)^2 \ln\left(1-\frac{2}{q}\right)\Big]. \end{aligned} \tag{D.1}$$

$J(q)$ has the properties

$$\begin{aligned} J(q\to 0) \ &=\ \pi(1-\ln 2)\ q - \frac{\pi}{48}\ q^3 + \cdots, \quad J(q\to\infty) = \frac{4\pi}{3}\left(\frac{1}{q^2} + \frac{8}{15}\frac{1}{q^4} + \cdots\right), \\ J(2) \ &=\ \frac{4\pi}{3}(1-\ln 2), \quad J'(2^+) = -\frac{\pi}{3}(-1+4\ln 2), \quad J'(2^-) = -\frac{\pi}{6}(-5+8\ln 2). \end{aligned} \tag{D.2}$$

(Notice $I(q\to 0) = \frac{8\pi}{3}J(q\to 0)$.) $J(q)$ has a maximum of 1.3 at $q = 1.9$. $J(q)$ is continuous at $q = 2$, but $J'(q)$ has there a jump discontinuity. Its normalization is

$$\int_0^\infty dq\ J(q) \ =\ \frac{\pi}{9}(-3+\pi^2+6\ln 2). \tag{D.3}$$

$J(q)$ is shown in Fig. 10. Multiplying the integral

$$\int_0^\infty \frac{dq}{q^2}\ [J(q) - \pi(1-\ln 2)\ q\Theta(1-q)] \ =\ \frac{\pi}{8}[10-\pi^2+8(1-\ln 2)\ln 2] \approx 0.719405 \tag{D.4}$$

with $-2/\pi^3$ yields (3.13).

The original expression for $J(q)$ arises from the diagram rules for $\Sigma_{2\mathrm{d}}$ with Eq. (3.3) as

$$J(q) = \mathrm{Re}\int d^2e \int \frac{d\eta}{2\pi\mathrm{i}} Q(q,\eta) \left[\frac{\Theta(|\boldsymbol{e}+\boldsymbol{q}|-1)}{\boldsymbol{q}(\boldsymbol{e}+\frac{1}{2}\boldsymbol{q})-\eta-\mathrm{i}\delta} + \frac{\Theta(1-|\boldsymbol{e}+\boldsymbol{q}|)}{\boldsymbol{q}(\boldsymbol{e}+\frac{1}{2}\boldsymbol{q})-\eta+\mathrm{i}\delta} \right] \tag{D.5}$$

One way is to insert (A.4). It results [with $x_1 = \boldsymbol{q}(\boldsymbol{e}_1+\frac{1}{2}\boldsymbol{q})$, $x_2 = \boldsymbol{q}(\boldsymbol{k}_2+\frac{1}{2}\boldsymbol{q})$]

$$J(q) = \int \frac{d^2e_1}{4\pi} d^3k_2 \left[\frac{\Theta(|\boldsymbol{e}_1+\boldsymbol{q}|-1)\ P}{x_1+x_2} + \frac{\Theta(1-|\boldsymbol{e}_1+\boldsymbol{q}|)\ P}{x_1-x_2} \right] \Theta(1-k_2)\Theta(|\boldsymbol{k}_2+\boldsymbol{q}|-1) \tag{D.6}$$

in agreement with Eq. (3.4). Another way is the deformation of the integration contour from the real to the imaginary axis with $\eta = \mathrm{i}qu$. It yields

$$J(q) = \int_0^\infty du \left[\ln \frac{u^2+(1+\frac{q}{2})^2}{u^2+(1-\frac{q}{2})^2} \right] R(q,u) \tag{D.7}$$

as an integral identity.

Comparing $J(q)$ with $I(q)$:

$$\int_0^\infty \frac{dq}{q^2} \left[\frac{3}{8\pi} I(q) - J(q) \right] = \frac{\pi^3}{3} a\ . \tag{D.8}$$

Note $\frac{3}{8\pi} I(q \to 0) = J(q \to 0) = \pi^3 aq$. The identity (D.8) leads to the sum rule (3.15).

Figures

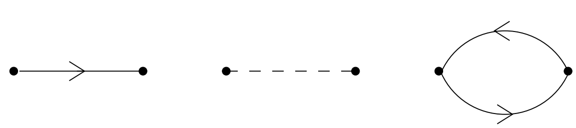

FIG. 1: Feynman diagrams for the one-body Green's function of the ideal Fermi gas $G_0(k,\omega)$, the bare Coulomb repulsion $v_0(q)$, and the RPA polarization propagator $Q(q,\eta)$ as defined in Eqs. (A.2)-(A.4).

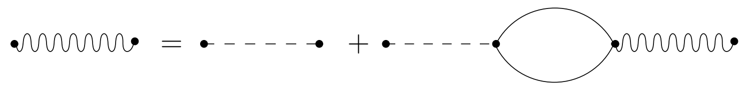

FIG. 2: Feynman diagrams for $v_{\mathrm{r}} = v_0 + v_0 Q v_{\mathrm{r}}$, the screened Coulomb repulsion in RPA.

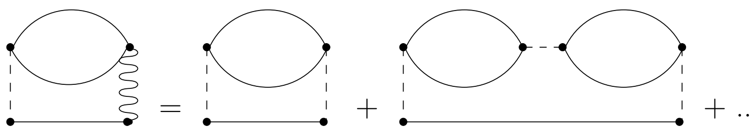

FIG. 3: Feynman diagrams for the ring-diagram-summed self-energy $\Sigma_{\mathrm{r}} = G_0 \cdot (v_{\mathrm{r}} - v_0)$ as defined in Eq. (3.4).

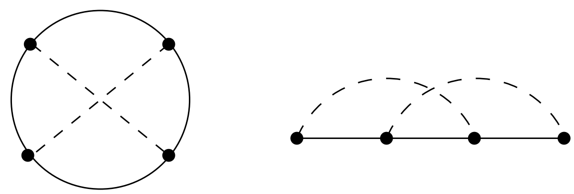

FIG. 4: Feynman diagrams for $e_{2\mathrm{x}}$ [11] and $\Sigma_{2\mathrm{x}}$ [20].

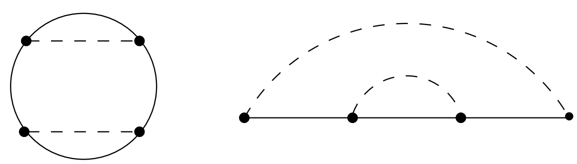

FIG. 5: Feynman diagrams, which do not contribute to e_2 and Σ_2, respectively.

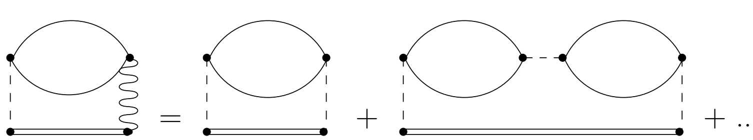

FIG. 6: Feynman diagrams for $\Sigma_{\mathrm{r}}^{\mathrm{x}} = G_{\mathrm{x}} \cdot (v_{\mathrm{r}} - v_0)$. For G_{x} see Fig. 7 and Eq. (3.14)

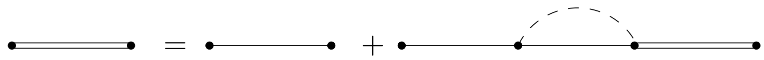

FIG. 7: Feynman diagrams for the renormalized one-body Green's function $G_{\mathrm{x}} = G_0 + G_0 \Sigma_{\mathrm{x}} G_{\mathrm{x}}$, see Eq. (3.14).

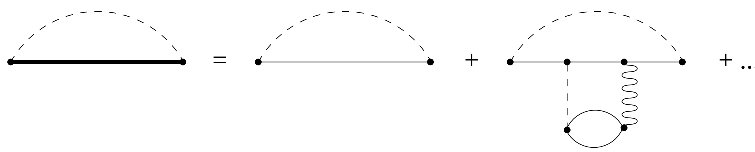

FIG. 8: Feynman diagrams for $\Sigma^{\mathrm{HF}} = G v_0$ with G = full one-body Green's function of the interacting system, $G = G_0 + G_0 \Sigma G$, Σ = full self-energy. The lowest-order term is $\Sigma_{\mathrm{x}} = G_0 v_0$, therefore the correlation part is $\Sigma_{\mathrm{c}}^{HF} = (G - G_0) v_0$.

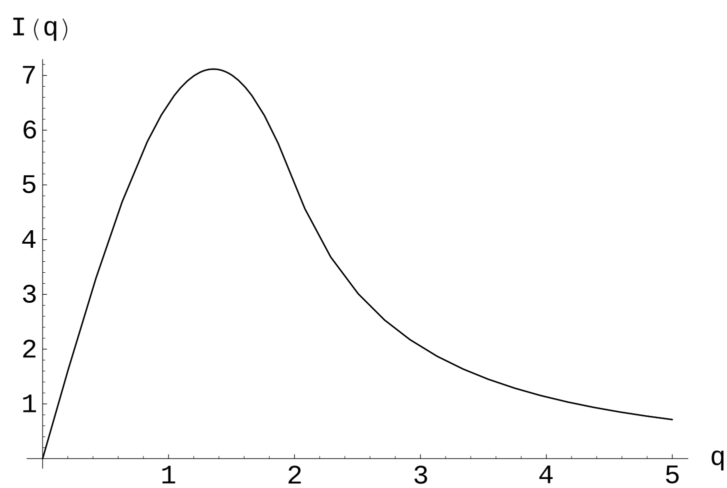

FIG. 9: The Macke function $I(q)$ according to Eq. (C.1), $I(q \to 0) = \frac{8\pi^4}{3} a q$.

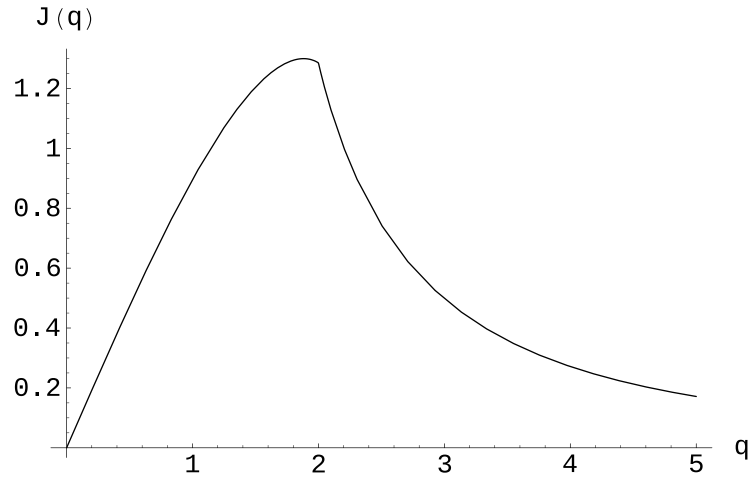

FIG. 10: The function $J(q)$ according to Eq. (D.1), $J(q \to 0) = \pi^3 aq$.